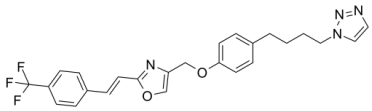
Data Sheet

Product Name:	Mubritinib
Cat. No.:	CS-3954
CAS No.:	366017-09-6
Molecular Formula:	C25H23F3N4O2
Molecular Weight:	468.47
Target:	EGFR
Pathway:	JAK/STAT Signaling; Protein Tyrosine Kinase/RTK
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : 50 mg/mL (106.73 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Mubritinib (TAK-165) is a potent and selective **EGFR2/HER2** inhibitor with an **IC_{50}** of 6 nM. IC50 & Target: IC50: 6 nM (EGFR2)[1] **In Vitro:** Mubritinib (TAK-165) specifically inhibits HER2 tyrosine kinase with an IC_{50} 6 nM and does not inhibit other types tyrosine kinase up to 25 000 nM. Mubritinib inhibits HER2 phosphorylation and its down-stream Akt and MAPK in HER2 strongly expressing cells (BT474 breast cancer cell line). Mubritinib sensitivity depends on HER2 levels of each cell line. Especially, BT474 cells which over-express HER2 strongly is highly sensitive (IC_{50}=0.005 μM) and PC-3 cells which express HER2 very weakly is less sensitive (IC_{50}=4.62 μM). But, HT1376 and ACHN cells that over-expressed EGFR showed high IC_{50} (IC_{50}>25 μM)[1]. **In Vivo:** In the xenograft model, treatment with Mubritinib (TAK-165) significantly inhibits growth of UMUC-3, ACHN, and LN-REC4. The antitumor effect after 14 days treatment are 22.9%, 26.0%, and 26.5% in UMUC3, ACHN and LN-REC4, respectively[1].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: [1]Cells are treated with Mubritinib at various concentrations (5 nM-25 μM) for 72 h. After the incubation period, the cells are counted. The IC_{50} value is calculated from a dose-response curve generated by least-squares linear regression of the response[1].
Animal Administration: [1]Mice: UMUC-3 and LN-REC4 cells are implanted with 50% Matrigel solution. After the tumor volume reaches 200–300 mm^3 in LN-REC4 and UMUC-3 cells and to 100–200 mm^3 in ACHN, the mice are treated orally twice daily for 14 days with vehicle (control) or 10 or 20 mg/kg per day of Mubritinib[1].

References:

[1]. Nagasawa J, et al. Novel HER2 selective tyrosine kinase inhibitor, TAK-165, inhibits bladder, kidney and androgen-independent prostate cancer in vitro and in vivo. Int J Urol. 2006 May;13(5):587-92.

CAIndexNames:

1H-1,2,3-Triazole, 1-[4-[4-[[2-[(1E)-2-[4-(trifluoromethyl)phenyl]ethenyl]-4-oxazolyl]methoxy]phenyl]butyl]-

SMILES:

FC(C1=CC=C(/C=C/C2=NC(COC3=CC=C(CCCCN4N=NC=C4)C=C3)=CO2)C=C1)(F)F

Caution: Product has not been fully validated for medical applications. For research use only.

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